Efficient Computerized Model for Dynamic Analysis of Energy Conversion Systems

R. D. Hughes, F. L. Lansing, and I. R. Khan
DSN Engineering Section

In searching for the optimum parameters that minimize the total life cycle cost of an energy conversion system, one must examine various combinations of components and study the resulting system performance and associated economics. The Systems Performance and Economics Simulation computer program (SPECS) was developed to fill this need. The program simulates the fluid flow, thermal, and electrical characteristics of a system of components on a quasi-steady-state basis for a variety of energy conversion systems. A unique approach is used in which the set of characteristic equations is solved by the Newton-Raphson technique. This approach eliminates the tedious iterative loops which are found in comparable programs such as TRNSYS or SOLTES-1. Several efficient features were also incorporated such as the centralized control and energy management scheme, the analogous treatment of energy flow in electrical and mechanical components, and the modeling of components of similar fundamental characteristics using generic subroutines. Initial tests indicate that this model can be used effectively with a relatively small number of time steps and low computer cost.

I. Introduction

The satisfactory development and design of efficient and economical energy conversion systems require a thorough understanding of the interactions of the energy sources, system components, exterior environment, load distribution and automatic control devices. It is necessary to select components from among many proposed configurations that vary widely in performance characteristics and affect the overall system cost. Since experiments on new configurations are expensive and time-consuming, properly formulated computer simulations can provide the same information at much less time and cost.

As part of the continuing engineering efforts to upgrade the performance of the NASA-owned antenna facilities of the Deep Space Network (DSN) at JPL, it is desirable to obtain not only efficient "working" solutions but also "optimized" ones that minimize total system cost. Two steps should be taken in order to obtain optimum solutions. First, for a given energy conversion system configuration, the optimized performance parameters must be determined. Because the design configurations of components are often extensive (Ref. 1), some bounds and size limits should be set on these parameters. Reliability and availability constraints are also added. Energy conservation measures, which reduce the energy consumption of the facility and subsequently affect

its operation and maintenance costs, must also be taken into account. Second, tradeoff studies of several optimized configurations must be made to select the optimum one.

At the supply side of an energy conversion system, energy is generated from a set of power plants; at the demand side, the energy is distributed among facility loads. It is essential, therefore, to match and balance, with minimum energy losses, the flow of energy between the generation and distribution sides. With the above energy balance, reliability, and cost constraints in mind, a detailed dynamic (i.e., time-varying) simulation of energy conversion systems is needed to analyze the system behavior and costs on a time-dependent basis.

It is common in system design to select equipment by assigning single values of key properties (such as pressures, temperatures, flow rates, voltages, currents, etc.) at critical network stations and select the appropriate size of components that meet given specifications. The more efficient dynamic simulation model, in contrast, assumes that the system configuration is defined, that all component sizes are selected and that the performance characteristics of all components are known. The simulation model then computes the station properties (pressures, temperatures, flow rates, voltages, and currents) at other than design loads. The model hence suits the following purposes:

(1) It can be used as an analytical tool for equipment design for large energy conversion systems where the cost of computer simulation represents a small portion of the total cost. The program can assist the designer in avoiding oversized or undersized systems and in selecting optimum equipment size. After completing a trial component selection based on one set of loadings, one can apply the model to other partial or overloading conditions to determine if the original design is adequate.

(2) It serves as a basis for developing "short cut" techniques after making a large number of detailed simulations on many different designs. These shorter solutions can be helpful in making initial assessments.

(3) It provides the field operator with a learning and diagnostic aid for understanding the dynamic performance of the operating system and the interrelationships between components at off-design conditions.

(4) It can be used to study the effects of add-on components and analyze the corrections sought for some operating problems if an existing system is expanded or reconfigured. The benefits of any modification can be assessed by analyzing the simulation results before and after making a change.

II. Survey of Existing Programs

A. Selection Criteria

The need to have such a time-varying simulation model has been encountered in many facility projects. The criteria described below are used in selecting the proper computer model in our literature search:

(1) The model should be a well-documented and low cost tool with an easily understood input, incorporating basic and fundamental analytical expressions, and thereby being available to a wide variety of users.

(2) The model should be modular and open-ended to simulate either small or large problems. The system size is determined by its number of components, and the model therefore should accommodate systems with arbitrary arrangements of series and parallel branches and have no limitations on these arrangements.

(3) The model should have the capability to simulate steady-state conditions for a system without capacitive components as well as quasi-steady-state conditions for a system with capacitive components (such as storage tanks, batteries, etc.). Quasi-steady-state simulation is done with time steps that are much larger than the largest time constant of all components. A true transient simulation involves time steps that are smaller than the smallest characteristic time constant of all components. A true transient simulation should be avoided since most of the components encountered in facility energy conversion systems, excluding capacitive components, respond to abrupt changes in local conditions in a relatively short time. This time response varies from a few seconds to several minutes, which makes computations using large time steps (such as every half-hour or every hour) suitable for quasi-steady-state conditions. The quasi-steady-state approach reduces the computation time tremendously without a significant loss of accuracy (Refs. 2, 3).

(4) The model should treat mechanical and electrical components in an analogous fashion. Examples are: a fluid pump vs an electrical generator, a pipe vs a connecting cable, a fluid storage tank vs a battery, etc. This analogous treatment will simplify the energy management and control schemes and reduce computer costs.

(5) The model should have a central monitor and control software, as in real systems, to monitor changes in the system parameters and send the appropriate signals to respond to internal constraints as determined by the component's behavior or to external controls imposed by the user.

The validity of any program depends primarily upon the formulation of the equations which it solves. Fundamental laws and relations such as energy balances, momentum balances, mass balances, and properties of substances in combination with the performance characteristics of components must all be written in the proper form. In general, one method of solving the equations is not necessarily as effective as another in saving time and computer cost. Among the many programs written in system dynamics the following ones are examined.

B. Available Programs

A detailed literature search showed that several computer programs which have been written for the dynamic simulation of solar-powered energy systems are relevant. TRNSYS (Ref. 4) for example, was developed by the University of Wisconsin to simulate solar-powered water heating and cooling systems. Sandia Laboratories, Albuquerque, New Mexico, has developed SOLSYS (Ref. 5), which is similar to TRNSYS but also includes simple Rankine-power cycles. Sandia later on developed SOLTES-1 (Simulator of Large Thermal Energy Systems (Ref. 6)), which is a combined version of SOLSYS and TRNSYS. SOLTES-1 simulates, in a modular approach, Rankine-power cycles, solar powered heating and cooling systems. Though flexible and modular, TRNSYS and SOLTES-1 are limited to solar-powered systems only.

Other dynamic models such as LASL and CAL-ERDA were developed by Los Alamos Scientific Laboratory (LASL), Los Alamos, New Mexico (Ref. 7). These are limited also to the dynamic description of a double-glazed flat-plate solar-collector, a hot water energy storage, an absorption water chiller, an air-handler, and a building shell and its interior loads for solar-heated and solar-cooled buildings.

In computer hardware real-time simulation, the Utility Systems Group at JPL (Ref. 8) has developed an Electric Power System Simulator (EPSS) for the U.S. Department of Energy (DOE) Office of Electric Energy Systems, which is coordinated with NASA's Energy Systems Division. The simulator is a microprocessor-based device which is designed to illustrate the complexities of operating a real utility power system that consists of several combinations of electrical power generation units. It is a portable, table-top device consisting of display and video monitors portraying the total system performance for different combinations of energy generation, energy storage, and load-varying effects. Costs of energy are user-provided for each component according to the load curves and operating characteristics.

W. Stoecker at the University of Illinois, Urbana-Champaign, (Ref. 2), has developed a dynamic simulation using a different approach for centralized chilled water circuits. He has combined the Newton-Raphson technique for solving nonlinear pressure balance equations with a simple Gaussian elimination technique for solving linear heat-balance equations. The extension of this approach to complex energy conversion systems employing phase-change fluids was not tried elsewhere, although it is worth investigating because of its simplicity and time-saving potential.

In addition to the above programs, other models were developed by independent groups: DYNSIM by Honeywell Energy Resources Center, Minnesota (Ref. 9), SOLCOST by Martin Marietta Corporation, Colorado, HISPER by NASA's Marshall Space Flight Center (MSFC), Alabama, and STEPS by Colorado State University, Colorado (Ref. 10). Differences in accuracies of modeling a given problem have varied from +2% to +20% (Ref. 11), which shows the need for program unification and standardization.

After comparing the above available computer programs with their differences regarding handling of equations, completeness of documentation, operating time and cost, complexity of input data, and ability to be reconfigured to accommodate additional components, it was decided that writing a new program instead of modifying an existing one was necessary in order to obtain an engineering tool which would have the desired capabilities and efficiency. The Systems Performance and Economics Simulation Program (SPECS) was developed to fill this need. This article describes the following aspects of the SPECS computer program: the method used for modeling a system of components, the mathematical representation of these components, the numerical technique used in solving the resulting system of equations, and the program input and output.

III. Modeling Theory

Since an energy conversion system is a set of components interconnected to accomplish a specific task, it is by definition modular. It is possible to simulate its performance by collectively simulating the performance of its components. A large problem can be reduced to a number of smaller problems, each of which can be solved independently. Mathematically, the problem consists of constructing a set of nonlinear equations and solving these equations simultaneously using the Newton-Raphson technique instead of the commonly used consecutive approach. This approach avoids iteration of configurations with cyclic (closed loops), acyclic (open ended) and multicyclic (joint loops) calculations. The simultaneous solution process is repeated at each "selected" time step during a representative day of each month in the simulation period. A detailed economic analysis of the system follows its performance evaluation to establish a base for further optimization study. Additional features of the program are presented in the remainder of this section.

A. Definitions

It is necessary to define the terms "station," "streamline," and "component," since each has a definite meaning in the program description.

A "station" is a unique position on the electrical or fluid network. A station is defined by 2-digit integers (e.g., 27); a maximum of 99 stations can be defined.

A "streamline" is the path of energy (or fluid) flux between two adjacent stations. A streamline is identified by two stations, one upstream and one downstream.

A "component" is the smallest constituent of the system which performs a well-defined physical function when assembled with other components. Components as shown in Fig. 1 can be simple, with one streamline (one inlet station and one outlet station) or compound, with two or more streamlines (one or more inlet stations and one or more outlet stations). Components are distinguished by two identifiers and described by a set of performance parameters. The first identifier is for the component "type" which is a 2-digit integer (a maximum of 99 types could be identified) specifying whether the component is a pump, a pipe, a 2-way valve, a water tank, a heat exchanger, a wind turbine, etc. The second identifier is a component "position" identifier giving the relative component location in the system and its associated links with other stations and streamlines. No two components can have the same position identifier. A particular component type can appear in more than one place as needed to complete the function of the system. Additional component description parameters include size and flow characteristics and efficiencies or control strategies as described by the program inputs.

B. Newton-Raphson Technique

The Newton-Raphson technique (Ref. 2) used in the SPECS program is based on the linear approximation of the set of nonlinear functions $[F(X)] = 0$ around the root $[X^*]$ such that

$$\left.\begin{aligned} f_1(X) &= f_1(x_1, x_2, \cdots, x_N) = 0 \\ &\vdots \\ f_N(X) &= f_N(x_1, x_2, \cdots, x_N) = 0 \end{aligned}\right\} \quad (1)$$

or in matrix form:

$$\begin{aligned} [F] &= [f_1, f_2, \cdots, f_N] \\ [X] &= [x_1, x_2, \cdots, x_N], \end{aligned} \quad (2)$$

where $[X]$ is the vector of unknown variables. The Jacobian matrix $[J]$ is the "slope" matrix whose element J in the ith row and jth column is the derivative

$$J_{ij} = \partial F_i / \partial x_j \quad (3)$$

At the nth iteration the Taylor series expansion for $[F]^{(n)}$ around $[X]^{(n)}$ gives the following matrix equation:

$$[F]^{(n+1)} - [F]^{(n)} = \left[\frac{\partial F}{\partial x}\right]^{(n)} \{[X]^{(n+1)} - [X]^{(n)}\}$$

$$+ 0\,[\Delta X]^2$$

By truncating the series to drop terms of the order ΔX^2 and higher and evaluating the derivative matrix at the nth iteration

$$[F]^{(n+1)} - [F]^{(n)} \cong [J]^{(n)} \{[X]^{(n+1)} - [X]^{(n)}\} \quad (4)$$

or

$$[X]^{(n+1)} \cong [X]^{(n)} + [J]^{-1(n)} \{[F]^{(n+1)} - [F]^{(n)}\} \quad (5)$$

At an $(n+1)$th iteration, which is assumed to bring the trial $[X]^{(n+1)}$ close to the root $[X^*]$, the function $F^{(n+1)}$ approaches zero and the non-zero residual ($[F]^{(n)}$) is used to obtain the updated value of $[X]^n$. Equation (5) then gives:

$$[X]^{(n+1)} \cong [X]^{(n)} - [J]^{-1(n)} [F]^{(n)} \quad (6)$$

Note that if $[X]^{(n)} \neq [X^*]$, the function set $[F]^{(n)}$ will not equal zero, rather, it equals a "residual" which tends to be close to zero as the iteration proceeds. Instead of inverting the Jacobian matrix, a modified Gauss-Jordan elimination technique is used to solve Eq. (6).

Convergence is accepted when the condition:

$$|\,[X]^{(n+1)} - [X]^{(n)}\,| \leqslant [\epsilon] \quad (7)$$

is met or when n exceeds a user-specified upper limit. The value of the variable $[X]$, computed at the end of one time step, is used as the initial guess for the iteration at the next time step and the above process is repeated until the simulation period is completed.

Note that the variables sought at the end of each time step can be classified as (a) "equilibrium" variables that are free to take on any value during the time step and therefore they are determined by the program after satisfying all conservation

laws, and (b) externally controlled (or source/sink) variables that must be kept at a fixed value during each iteration step as determined by the user's input controls. The structure of the Jacobian matrix includes only the first type of variables.

C. Equations and Unknowns in a Fluid Network

The set of nonlinear equations needed to describe a fluid network can be obtained by characterizing each fluid station in the fluid network by a vector $[V]$ which is composed of seven elements:

$$[V] = [\dot{m}, P, h, T, \mathrm{v}, s, x] \tag{8}$$

where $\dot{m}$ is the fluid mass flow rate, P is the absolute pressure, h is the specific enthalpy, T is the absolute temperature, v is the specific volume, s is the specific entropy, and x is the quality (or dryness fraction). These seven fluid properties constitute $7S$ unknowns for a fluid network that consists of S number of fluid stations. Energy is transferred across the boundary of each component in the network in three possible forms: heat, $\dot{Q}$; electrical work, $\dot{W}_e$; and mechanical (or shaft) work, $\dot{W}_m$; thus adding $3C$ unknowns for C components. The $(7S + 3C)$ equations needed to solve these $(7S + 3C)$ unknowns are grouped as follows:

(1) For each fluid station where the fluid is a pure substance, only two independent thermodynamic properties are needed out of the six properties: p, h, T, v, s, and x. The thermodynamics-property subroutines are designed to compute the remaining four thermodynamic properties once two properties are specified. The property subroutines thus act as $4S$ implicit equations for a network of S fluid stations.

(2) The continuity and momentum equations form a set of $2(S - 1)$ equations for S fluid stations in a closed fluid loop. These equations are written along streamlines only. The number of equations depends upon the structure of the fluid network; two equations for each streamline minus two equations for closing the loop.

(3) If the first law of thermodynamics is applied to each component boundary or control volume, a maximum set of C equations for C components can be obtained. Additional component equations (equals $2C$) can be obtained from the second law of thermodynamics for the efficiency or effectiveness expressions and from the energy constraints for each component (such as no $\dot{Q}$, no $\dot{W}_e$, or no $\dot{W}_m$). A total of $3C$ equations are thus obtained.

(4) The remaining $(S + 2)$ equations can be written to control the properties at certain fluid stations by assigning values to temperature limits (for two-phase flows), pressure limits, quality limits, or mass flow limits. Control equations can be used to define load management as needed by the control software.

D. Structure of the Jacobian Matrix and Component Equations

Although the Jacobian matrix $[J]$ could take on various arrangements, the one sketched in Fig. 2 is one option. The elements $(\partial F_i / \partial x_j)$ are grouped so that the seven variables of the first fluid station are followed by the variables of the second station and so on until the Sth station is reached. Next to the station property variables, the derivatives of three variables $(\dot{Q}, \dot{W}_e, \dot{W}_m)$ of the first component are placed, followed by the three variables of the second component and so on until the Cth component is completed. Other arrangements can be adopted if found more advantageous.

Only components with a time constant much smaller than the iteration time step are included in the Jacobian structure since these components are treated as having Steady-State, Steady-Flow (SSSF) processes. Any capacitive component with a large time constant (such as a fluid storage tank) will be dealt with separately at the end of each time step, where the component is treated as having Uniform-State, Uniform-Flow (USUF) processes.

To avoid having discontinuous function derivatives, especially for the $4S$ implicit thermodynamic relations, the SPECS program includes a special treatment explained as follows. Once two thermodynamic properties (p and v, say) are known at the nth iteration step, the other corresponding four properties (in this case: h, s, T and x) are determined by the thermodynamics property subroutine. These four properties are treated as "fixed" or constants throughout the $(n + 1)$th iteration step. At the end of the $(n + 1)$th iteration, new values for the two properties (p, v) are obtained and the process is repeated.

If a fluid property y is assigned a temporary constant value y_0, an equation can be written to reflect this process:

$$y - y_0 = 0 \tag{9}$$

Accordingly, the element $J(i, j)$ of the Jacobian matrix corresponding to ith equation and the jth fluid property will be equal to 1 and all the other elements in the ith row become zero. If desired, these fluid properties, which are assumed to be temporarily fixed, could be excluded from the set of unknown equilibrium variables in the Jacobian, hence reducing the size of the Jacobian matrix. Additional tests, however, are

still required to determine whether these fixed variables in equations similar to Eq. (9) may save computation time.

As an illustration of the structure of the Jacobian matrix, consider the continuity, momentum and energy equations written for a compound stationary component (σ) with multiple inlet stations (i) and outlet stations (o) as sketched in Fig. 3.

For USUF conditions, the continuity equation becomes:

$$\sum_i \dot{m}_i(t) - \sum_o \dot{m}_o(t) = \frac{m_\sigma(t+\Delta t) - m_\sigma(t)}{\Delta t} \quad (10)$$

The momentum - impulse vector equation at time t becomes:

$$\sum_i \dot{m}_i [U_i] + \sum_i [P_i A_i] - \sum_o [P_o A_o]$$

$$+ [m_\sigma g] + [R] = \sum_o \dot{m}_o [U_o] \quad (11)$$

where [ ] indicates a vector of multiple components. $[R]$ is a boundary-surface force which could be negative (as a friction force opposing the flow) or positive (as a result of forced agitation by a blower or a pump).

The energy equation is written as:

$$\dot{Q} + \sum_i \dot{m}_i \left(h_i + \frac{U_i^2}{2} + gZ_i\right) - \dot{W}_m - \dot{W}_e$$

$$- \sum_o \dot{m}_o \left(h_o + \frac{U_o^2}{2} + gZ_o\right)$$

$$= \frac{E_\sigma(t+\Delta t) - E_\sigma(t)}{\Delta t} \quad (12)$$

where E_σ and m_σ are the internal energy and retained mass of the control volume σ, and t is the time. Equations (10 through 12) are used for USUF components only. The velocity U could be further expressed in terms of the mass flow rate as:

$$U_i = v_i \dot{m}_i / A_i$$

$$U_o = v_o m_o / A_o$$

For SSSF components which appear in the Jacobian matrix, Eqs. (10) through (12) are reduced to the following:

Continuity equation:

$$\sum_i \dot{m}_i - \sum_o \dot{m}_o = 0 \quad (13)$$

Momentum equation for a streamline:

$$P_i - P_o - (a_0 + a_1 \dot{m} + a_2 \dot{m}^2) = 0 \quad (14)$$

where the pressure change (R/A) is expressed by a polynomial in $\dot{m}$, and a_0, a_1, a_2 are constants determined by the component type. Energy equation for a SSSF component or a control volume:

$$\dot{Q} + \Sigma_i m_i \left(h_i + \frac{U_i^2}{2} + gZ_i\right) - \dot{W}_m - \dot{W}_e$$

$$- \Sigma_o \dot{m}_o \left(h_o + \frac{U_o^2}{2} + gZ_0\right) = 0 \quad (15)$$

The coefficients derivatives of Eq. (13) appear in the Jacobian matrix as 1, corresponding to an inlet station mass flow rate, -1 to the outlet station mass flow rate, and zero otherwise. Other simple relations can be derived from Eqs (14) and (15) in a similar manner.

IV. Program Structure

The SPECS program is structured in a modular fashion which will allow future modification of any aspect of the program. It consists of four blocks: (1) an input block, (2) a library block, (3) a control block, and (4) an output block as shown in Fig. 4. The input block contains the user-provided data. The library block contains the subroutines which perform various analytical and numerical computations. The library block computes all parameters for a given system configuration according to the data and specifications given in the input block. The control block monitors and manages the flow of information, solves the system of nonlinear equations at each time step, and controls the computational stability requirements. The output block prints for the user the final performance and economics results of a specific system. Note that the output block is controlled by user options for short, intermediate, or detailed printout.

The program language is FORTRAN IV. Use of FORTRAN "NAMELIST" is made to classify the input data into groups of common feature. Descriptions of program blocks and subroutines are as follows:

A. Input Block

The input to the SPECS program is divided into seven major groups:

(1) System configuration data.

(2) Station properties data.

(3) Components characteristics data.

(4) Control data.

(5) Outdoor environment/site data.

(6) Energy loads data.

(7) Economics data.

Each group is further described below.

1. System configuration data. This group defines the number, the type and location of components, the number and location of inlet and outlet fluid stations, the number of streamlines, etc. This information is used by the program to set limits of DO loops and determine the size of the problem under study.

2. Station properties data. This group includes the type of working fluid at each station, externally controlled properties, initial conditions and setpoints. All the pressures are computed relative to a user-assigned pressure at a reference point. The program also allows for differences in elevation of each station above some arbitrary datum.

3. Component characteristics data. This group includes the diameter and equivalent friction length for pipes and joints, the head-flow rate curve for a pump, the heat transfer coefficient times surface area product for a heat exchanger, the coefficient of velocity for a fully open valve, etc.

4. General control data. This group includes the case title, convergence criteria for termination of program, the time-step, the total simulation period, the type of results to be printed out for the user and options to read weather and load data.

5. Outdoor environment/site data. This group includes outside air dry-bulb temperature, outside air wet-bulb temperature, relative humidity, dewpoint temperature, wind speed and direction, site latitude, site elevation, and solar radiation components (direct normal, diffuse, and ground reflected) as measured by a pyrometer or tracking pyrheliometer. A 24-hour profile for one representative day of each month is selected throughout a year's simulation. The solar radiation data can be taken from field measurements or otherwise simulated using the deterministic ASHRAE model (Ref. 12) which is built into the program.

6. Energy loads data. This group includes space and water heating load, space cooling load, lighting load and other electrical energy loads consumed by the facility. Water consumption data can also be included. Since it is impractical to run a large model for each hour of the 8760 hours of a year, an appropriate compactness is required to save computation time. Therefore, loads data for two representative days for each month are satisfactory; the first is a load profile for weekdays and the second is a load profile for weekends and holidays. Twenty-four hourly values for each representative day are required for energy loads.

7. Economics data. For detailed life cycle cost and cash flow analyses, this group includes the installation, operation, and maintenance costs of all components in the system, purchased energy costs, energy escalation rate, discount rate, and salvage values, in addition to preimplementation costs such as site preparation, surveying, study and design costs, etc.

B. Library Block

This block contains five sets of subroutines:

(1) Thermodynamic properties subroutines.

(2) Component description subroutines.

(3) Gauss-Jordan subroutine.

(4) Solar-radiation simulation subroutine.

(5) Life cycle cost and cash flow subroutine.

Each set is described as follows:

1. Thermodynamic properties subroutines. The driver routine for the thermodynamic properties computation is called by the Control Block to obtain values of fluid properties at any fluid station. This routine forms, from a library file, an array containing tables of saturation data only for each fluid used in the network being analyzed. The array does not contain data for all 16 fluids, listed in Table 1, which SPECS recognizes. This subroutine computes the values of four properties: (p, h, s and x), given the values of the two independent properties (T, v) for a fluid according to the flow chart in Fig. 5.

If the fluid is in the 2-phase saturated region ($v_f < v < v_g$) where the subscripts f and g denote saturated liquid and

saturated vapor, respectively, the driver routine computes the values of p, h, s, and x by interpolating according to T at constant v. If the fluid is in the compressed region ($v < v_f$), the four properties are calculated based on approximations using the saturated liquid conditions.

If the fluid is in the superheated region ($v > v_g$), general analytical expressions from Ref. 13 are used to calculate p, h, s, and x as a function of T and v. A set of fluid-specific subroutines calculates the two ideal gas properties (h^*, s^*) followed by the generalized expressions to compute the departure from ideal gas properties.

After the computation of all four properties is complete, the values are returned to the Control Block. Thus this subroutine acts as $4S$ implicit equations for a system having S number of fluid stations.

In addition to the six thermodynamic properties analyzed in this subroutine, three other physical properties are stored for each of the 16 fluids: the thermal conductivity, $k(T)$, dynamic viscosity, $\mu(T)$, and specific heat, $C_p(T)$. These three physical properties are given for both liquid and superheated vapor forms.

2. **Component description subroutines.** This set is a library of component model subroutines from which the user can draw to configure the specific system under study. The components are divided into generic categories according to function. Mass, momentum, energy conservation equations, and performance effectiveness relations can be written regardless of differences in design, operating conditions, and working fluids. These differences are taken into account by assigning different values for similar parameters in each component. This process eliminates superfluous component models of similar type.

For example, a counterflow recuperator, a parallel flow recuperator, and a heat regenerator could be simply grouped under one component type: a heat exchanger in which heat transfers from one medium to another. The distinct behavior of each component, however, is accounted for by different analytical expressions for the effectiveness, heat capacities of exchanging media, number of heat transfer units, and the conductance heat transfer area product.

Distinction between mechanical components is made based on the number of streamlines and inlet and outlet stations as shown in Fig. 1. Electrical components are modeled by simple relations between $\dot{W}_m$, $\dot{W}_e$, and $\dot{Q}$. Some of the generic component types to be modeled include but are not limited to the following:

(1) A heat exchanger (boiler, recuperator, and regenerator with phase change in one or two media).

(2) A fluid pump (rotary, screw, and positive displacement).

(3) A compressor (for air, refrigerant, etc.).

(4) A turbine (for steam, organic fluid, gas, wind, water).

(5) A simple heater (for air or water) or a simple cooler without phase change of either medium.

(6) A solar collector (flat plate, parabolic trough, paraboloid concentrator, etc.).

(7) A fluid storage tank (compressed air, water, steam accumulator, etc.).

(8) Electrical battery.

(9) Electrical motor.

(10) Electrical generator or alternator.

(11) Photovoltaic cell (flat plate or concentrated type).

(12) A mixing valve.

(13) A splitting valve.

(14) A pressure reducing valve.

(15) A fluid pipe (insulated or noninsulated).

(16) An underground cable or electrical transmission line.

(17) Building structure.

(18) Air-handler for air conditioning (dual duct, variable air volume type, etc.).

(19) A thermoelectric cell for power generation or refrigeration.

(20) A thermionic cell for power generation.

(21) A fuel cell.

(22) An absorption chiller (using lithium bromide-water, aqua-ammonia, etc.)

3. **Newton-Raphson iteration subroutine.** This subroutine solves the system of nonlinear equations using the Gauss-Jordan reduction method with diagonal pivoting instead of directly inverting the Jacobian matrix. This subroutine is written in double precision arithmetic to overcome the problem of oscillatory convergence during iteration.

4. **Solar radiation simulation subroutine.** Based on the deterministic model set by ASHRAE (Ref. 12), the total solar

radiation intensity (including the direct, diffuse, and ground-reflected components) falling on a surface is analytically simulated for the user's convenience. The solar elevation, azimuth, and declination angles are computed for 24 hours for one representative day of each month. The information available in this subroutine pertains to various solar collector types, selected as follows:

(1) Tilted flat plate, with arbitrary tilt angles.

(2) Horizontal flat plate.

(3) Single-axis tracking surface, with east-west orientation.

(4) Single-axis tracking surface with north-south orientation.

(5) Single-axis tracking surface with polar mount; i.e., the surface is oriented toward north-south line with a tilt angle to the horizontal which equals latitude.

(6) Two-axis tracking surface, always perpendicular to the sun's direct rays.

For northern latitudes, the surfaces are oriented toward the south, and for southern latitudes, toward the north. Additional surface configurations can be added in this subroutine provided they follow the SPECS format.

5. Life cycle cost subroutine. This subroutine calculates, for the system under study, the yearly maintenance and operation costs and the life cycle cost and presents a detailed cash-flow analysis. The methodology used in the subroutines follows the National Bureau of Standards' economic criteria as outlined in Ref. 14.

C. Control Block

This is the main routine which executes, monitors, controls and drives the whole program as sketched in Fig. 6. It enters the input data and sends the desired output. The main routine calls the thermodynamic properties subroutines in order to determine the properties of flow for each station. It also calls the set of component description subroutines to compute equation residuals and partial derivatives, which compose the Jacobian matrix, and executes the Newton-Raphson software to solve the system of nonlinear equations.

As in a real system, the control block is thought of as receiving input signals at the end of each iteration step, represented in the values of the variables (such as temperature, pressure, mass flow rate, etc.). It compares these input signals to one another or to set points and transmits the resulting "logical" signal to a logic element where a transformation occurs to generate output signals to actuators (represented by a set of analytical expressions or tabular data) for the operation of dampers, valves, pumps, boilers, etc.. A "truth-table" is another way of representing the function of the controller-actuator in handling the input/output signals in the simulation.

D. Output Block

The output of the program is controlled by several input variables. The computation results consist of the value of the different thermal and electrical loads at that particular hour, the thermo-dynamic properties at each station, the energy flux across each component of the system, and the overall performance, efficiency, and economics of the system. Several user options are introduced to obtain the desired level of printout detail.

V. Simulation Steps

The philosophy of the program logic can be visualized as an attempt to perform in a stepwise manner what the real system does in a continuous mode of operation following a startup. To simulate a particular system configuration, the major steps of program operation are as follows:

Step 1 (user's input data): After all input data are entered into the program, the user can "echo" or print-back all input data for rechecking.

Step 2: The dynamic simulation starts by the control block which groups the built-in characteristic equations of the components of the system being simulated. Because the Newton-Raphson method is iterative, it is essential to choose initial trial values of the variables to start iteration at each time step. Fluid valves can be initially set at their half-open position, and continuously adjusted as iteration proceeds. At the end of one time step, the results are used as the initial guess for iteration at the following time step, and so on. The above process is repeated until the simulation period has elapsed.

Step 3: The check for convergence is based on the changes occurring between one iteration step and the preceding step. If the changes in all the variables are less than a specified tolerance, $[\epsilon]$, the computation is considered convergent and the program proceeds to Step 5; otherwise the program proceeds to Step 4 for another iteration.

Step 4: Revise the initial setting of temperature and pressure controllers, valves, set points, etc. Diagnostic messages are printed if the variables attain unreasonable values or if convergence is not attained after a prescribed number of iterations. The program returns to Step 2 with updated values of the parameters.

Step 5: The program now prints out complete energy and flow rate profiles for the whole system under daily, monthly, and yearly operation. Detailed life-cycle cost and cash flow analyses are made over a given number of years.

Step 6: Additional optimization and parameter sensitivity will result from employing a search-type optimization technique at different design or operating conditions by repeating Steps 1 through 5.

VI. Program Summary

The SPECS program in its present form is structured to follow the above block descriptions. Current activities relate to the following:

(1) Incorporating a detailed economics package for the system life cycle costs and cash flow analysis.

(2) Improving and expanding the tabulated results in the output block.

(3) Expanding the components subroutines in the library block to include all the candidate components in Section IV-B-2.

(4) Debugging, testing, and documenting the final version of the program in order to extend its use to other design projects.

In summary, the SPECS model was developed to suit the following purposes:

(1) To be used as an analytical tool for equipment design for large energy conversion systems where the cost of computer simulation represents a small portion of the total cost.

(2) After completing a trial equipment selection based on one set of loadings, the designer can apply the model to other partial or overloading conditions to determine if the original design is adequate.

(3) To serve the basis for developing "short cut" techniques after making a large number of detailed simulations on many different designs.

(4) To provide the field operator with diagnostic aid for understanding the dynamics of the operating system and the relationships between components at off-design conditions.

(5) To study the effects of add-on components and analyze the corrections sought for some operating problems if an existing system is expanded or reconfigured.

The article has described these aspects of the SPECS computer program: the method used for modeling a system of components, the mathematical representation of these components, the numerical technique used in solving the resulting system of equations, and the program input and output.

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Table 1. List of fluids used in SPECS

Type No.	Fluid	Chemical symbol
1	Water	H_2O
2	Ammonia	NH_3
3	Helium	He
4	Hydrogen	H_2
5	Refrigerant 11 (trichlorofluoromethane)	CCl_3F
6	Refrigerant 12 (dichlorodifluoromethane)	CCl_2F_2
7	Refrigerant 13 (chlorotrifluoromethane)	$CClF_3$
8	Refrigerant 14 (carbontetrafluoride)	CF_4
9	Refrigerant 22 (chlorodifluoromethane)	$CHClF_2$
10	Refrigerant 23 (trifluoromethane)	CHF_3
11	Refrigerant 114 (dichlorotetrafluoroethane)	$CClF_2CClF_2$
12	Refrigerant 318 (octafluorocyclobutane)	C_4F_8
13	Refrigerant 500 (azeotropes (73.8/26.2))	CCl_2F_2/CH_3CHF_2
14	Refrigerant 502 (azeotropes (48.8/51.2))	$CHClF_2/CClF_2CF_3$
15	Refrigerant 503 (azeotropes (40.1/59.9))	$CHF_3/CClF_3$
16	Sodium	Na

List of Symbols

A	cross-section area
c_p	specific heat
C	number of SSSF components
f	function symbol
g	local acceleration of gravity
h	enthalpy
J	Jacobian matrix
k	thermal conductivity
l	streamline index
m	mass flow rate
n	iteration step index
N	number of unknown variables
P	absolute pressure
Q	heat rate
R	boundary force due to friction or forced agitation
s	entropy
S	number of fluid stations
T	absolute temperature
U	velocity
v	specific volume
V	vector of station properties
W	work energy
z	elevation above sea level (or arbitrary datum)
ϵ	error limit for convergence
μ	dynamic viscosity

Subscripts

i	inlet
o	outlet
m	mechanical
e	electrical

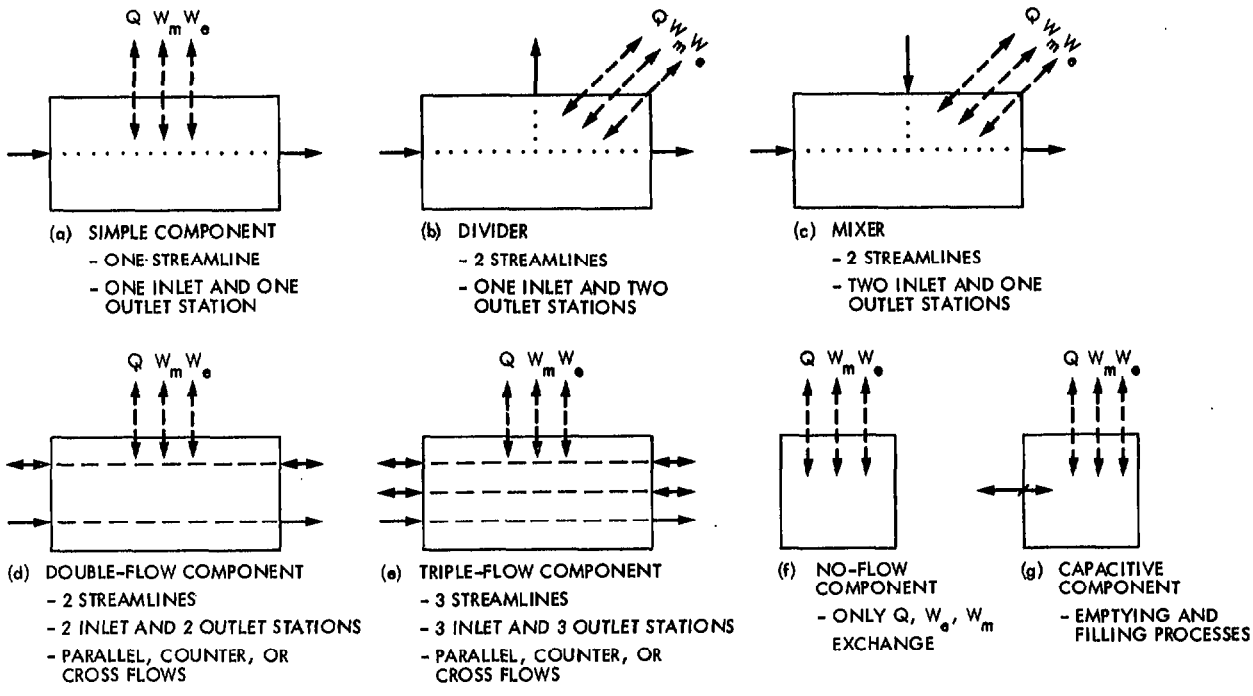

Fig. 1. Simple and compound components

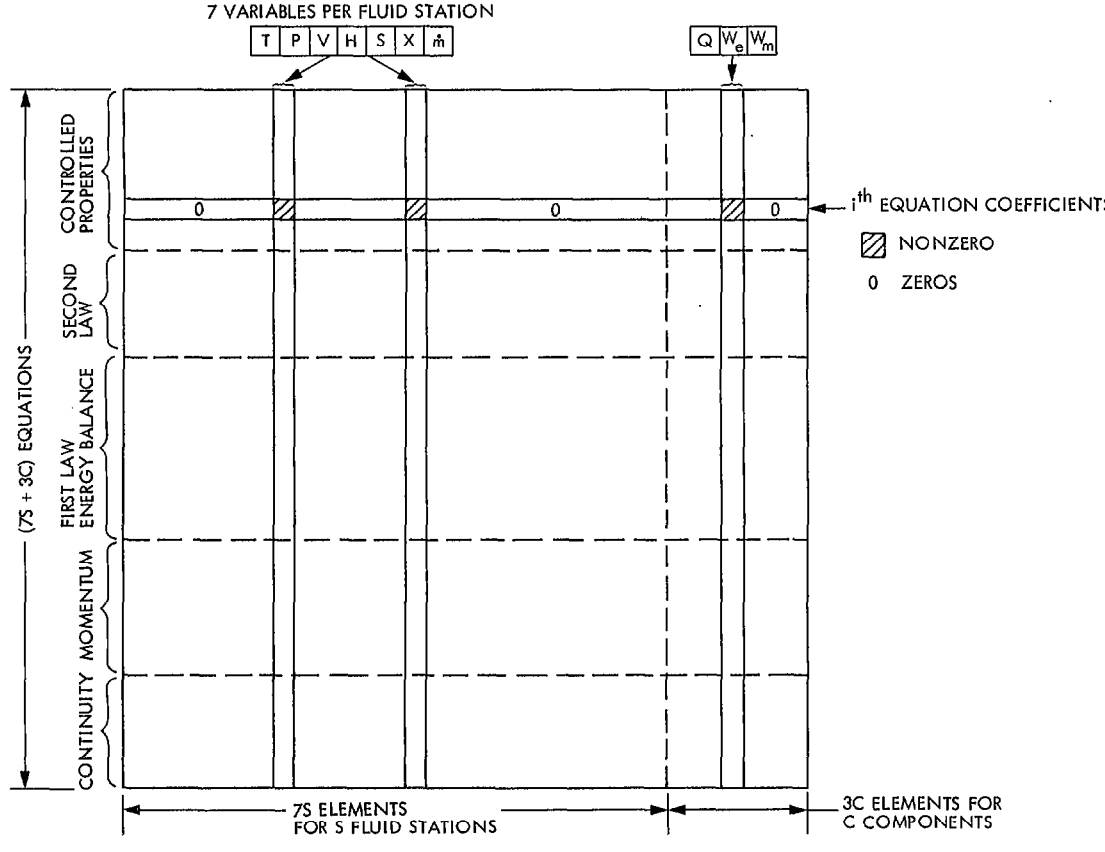

Fig. 2. Details of the Jacobian matrix [J]

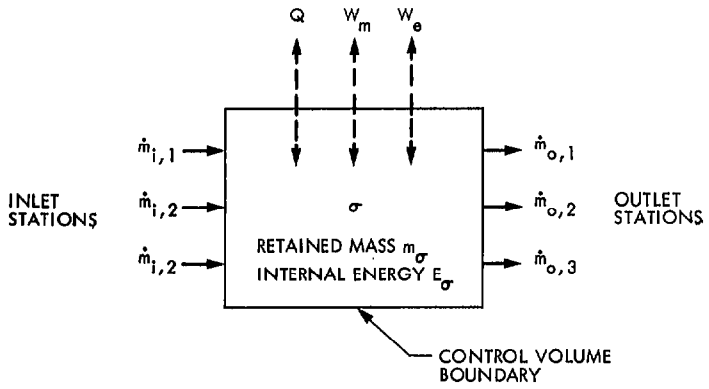

Fig. 3. Compound component σ with multiple inlet and outlet ports

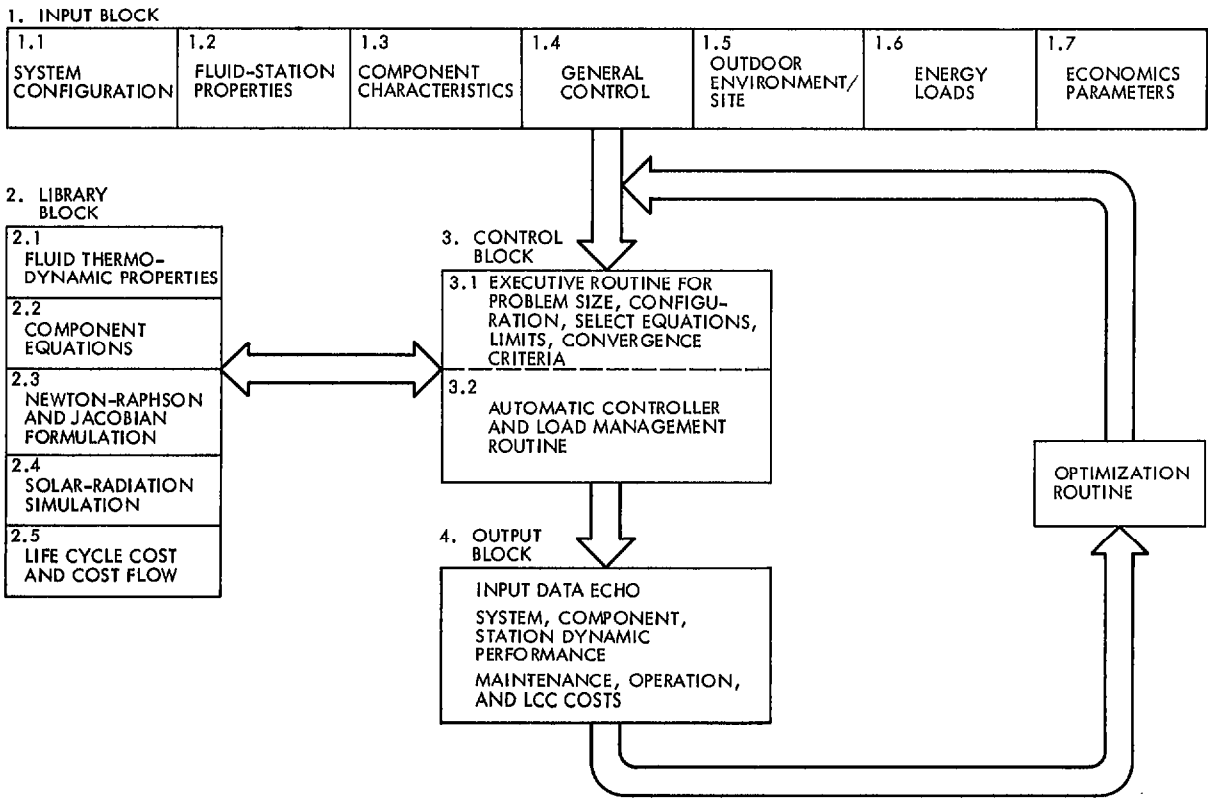

Fig. 4. Overall structure of SPECS program

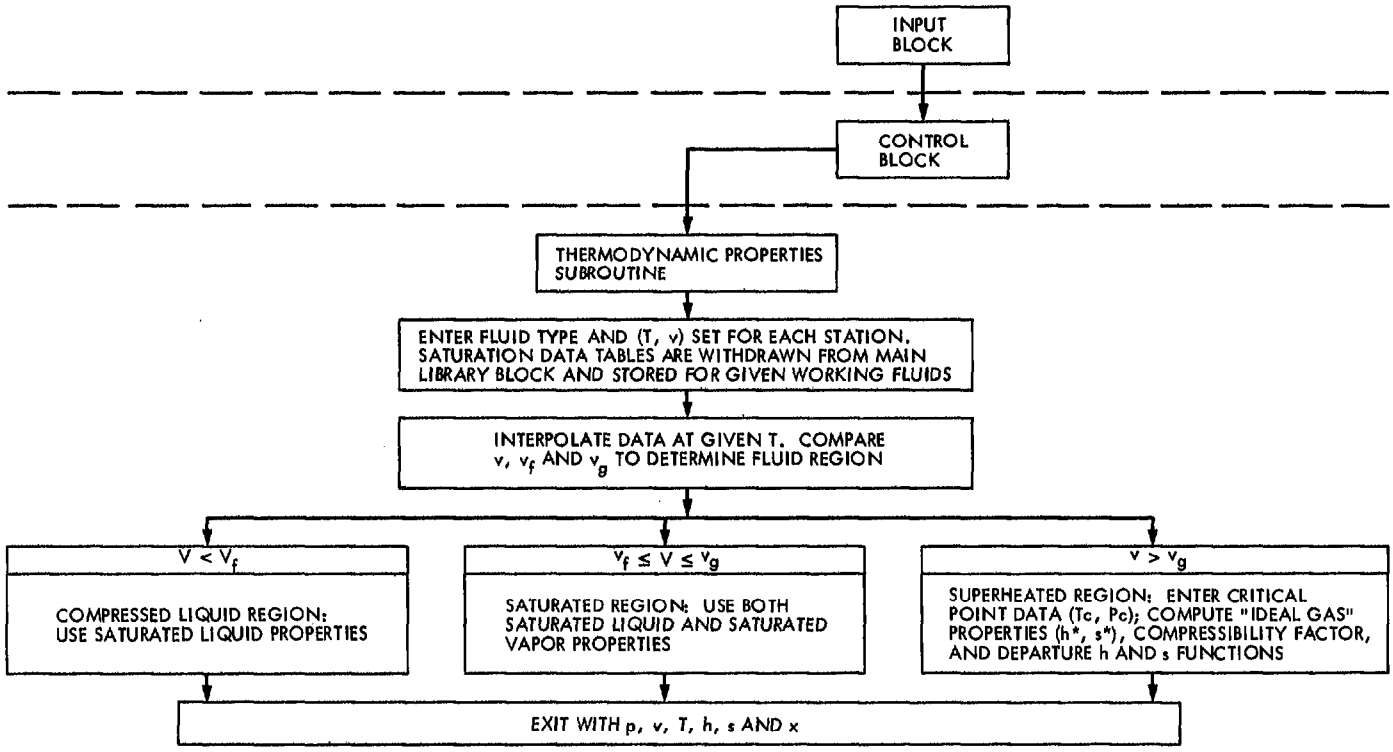

Fig. 5. Flow chart for thermodynamic properties subroutine

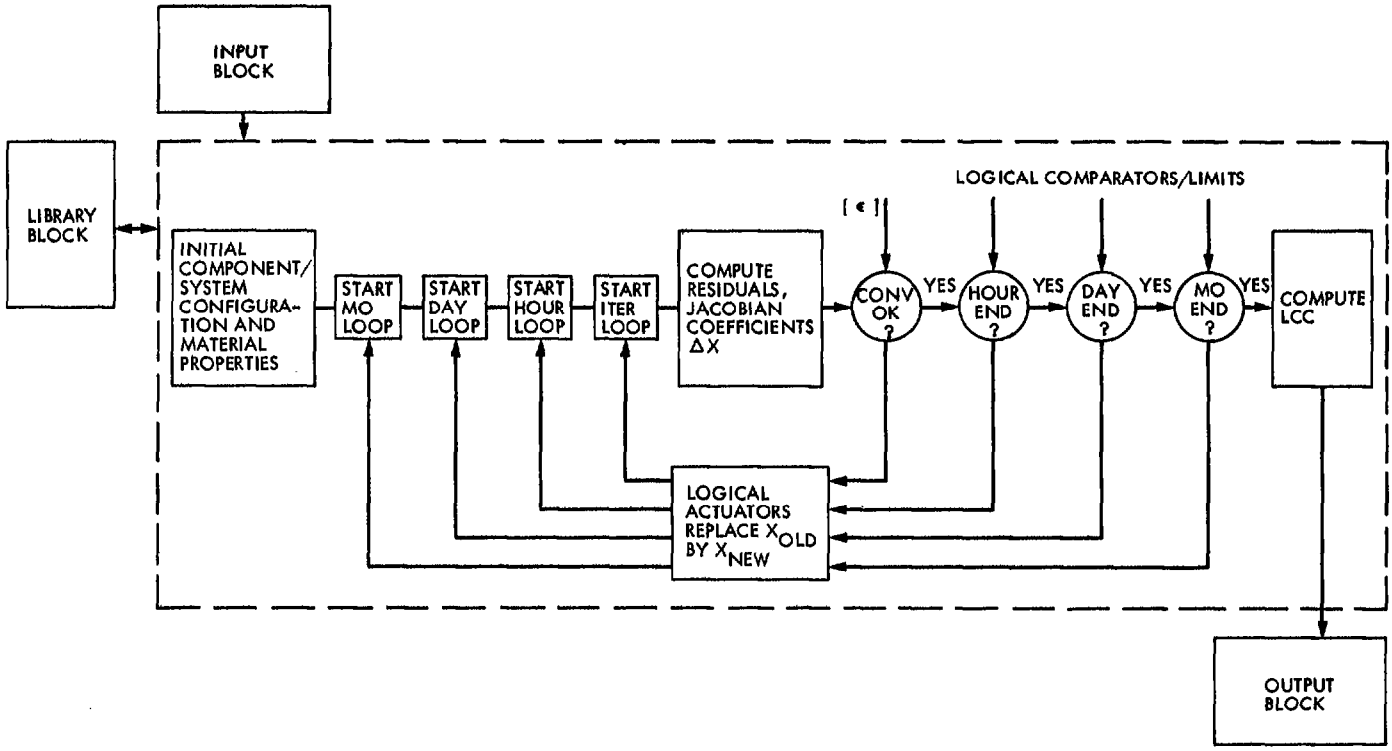

Fig. 6. Information flow in control block